

# Fuel Sulfur Conversion, Unburned Hydrocarbons and Impacts on Exhaust Composition

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## Questions:

- Are FSC data from fuel samples consistent with in-flight SO<sub>2</sub> emissions of the different fuels?
- Are there differences in total volatile aerosol emissions for Jet A and HEFA blend fuels?
- How do emission factors of selected hydrocarbons vary with engine thrust and fuel type?



# Airborne measurements used for this analysis

Compound	Instrument	Investigator	
SO <sub>2</sub>	Ion-Trap CIMS (CO <sub>3</sub> <sup>-</sup> )	Schlager / Klausner	(DLR)
H <sub>2</sub> SO <sub>4</sub>	Ion-trap CIMS (NO <sub>3</sub> <sup>-</sup> )	Schlager / Klausner	(DLR)
Hydrocarbons	AIMS CIMS (H <sub>3</sub> O <sup>+</sup> )	Voigt / Jurkat	(DLR)
Volatile CN	CPCs (5 nm, 10 nm)	Weinzierl / Sauer Anderson/ Moore	(DLR) (NASA)
CO <sub>2</sub>	CRDS NDIR Detcetor	Schlager Anderson	(DLR) (NASA)
NOx	CRDS	Anderson	(NASA)



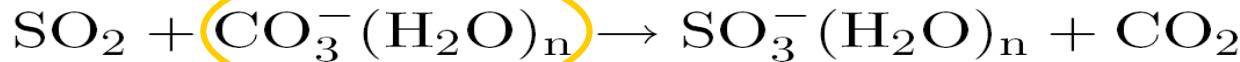
# Fuel sulfur content and sulfur conversion

- In-flight  $\text{SO}_2$  measurement technique and fuel sulfur content
- In-flight  $\text{H}_2\text{SO}_4$  measurement technique and gas-phase  $\text{H}_2\text{SO}_4$  in near-field plume
- Apparent volatile aerosol emission factors for Jet A and HEFA blend



# $\text{SO}_2$ IT-CIMS measurement technique

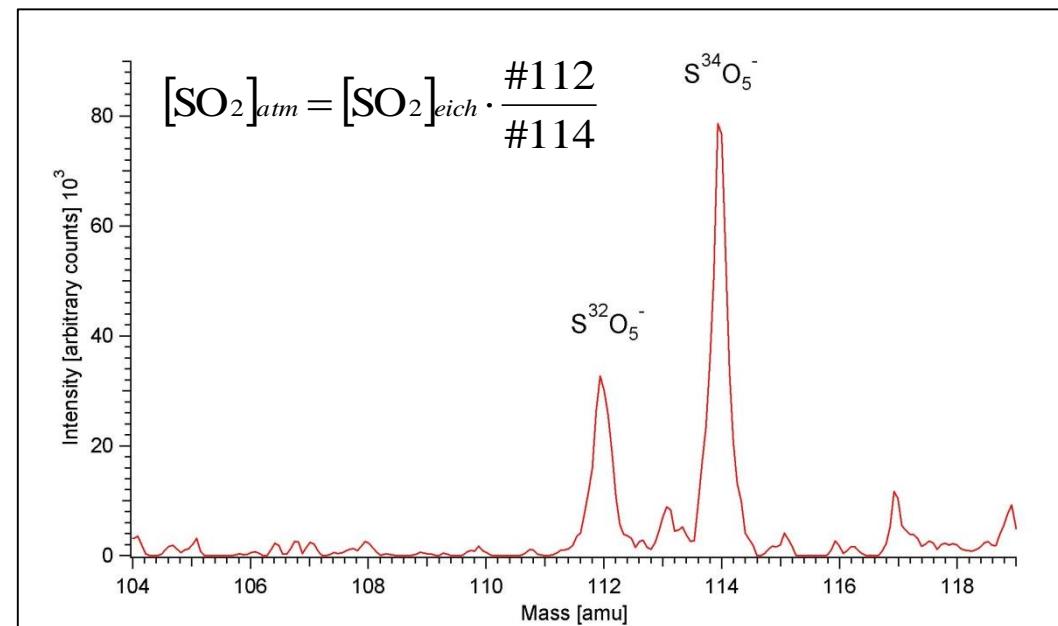
Educt ion



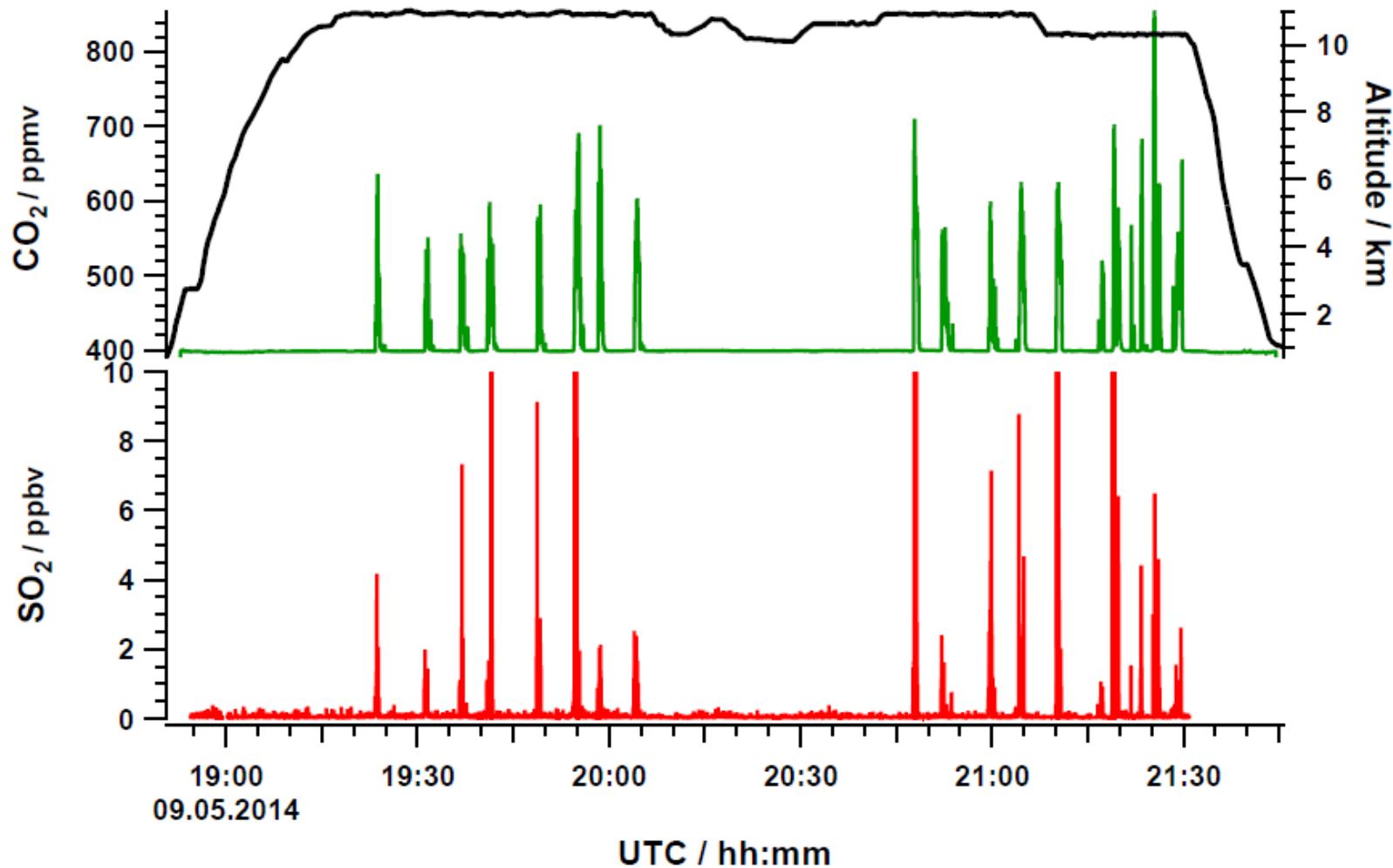
Product ion 112 amu

On-line calibration:  
Addition of isotopically  
labelled  $^{34}\text{SO}_2$  yields product  
ion with mass 114 amu

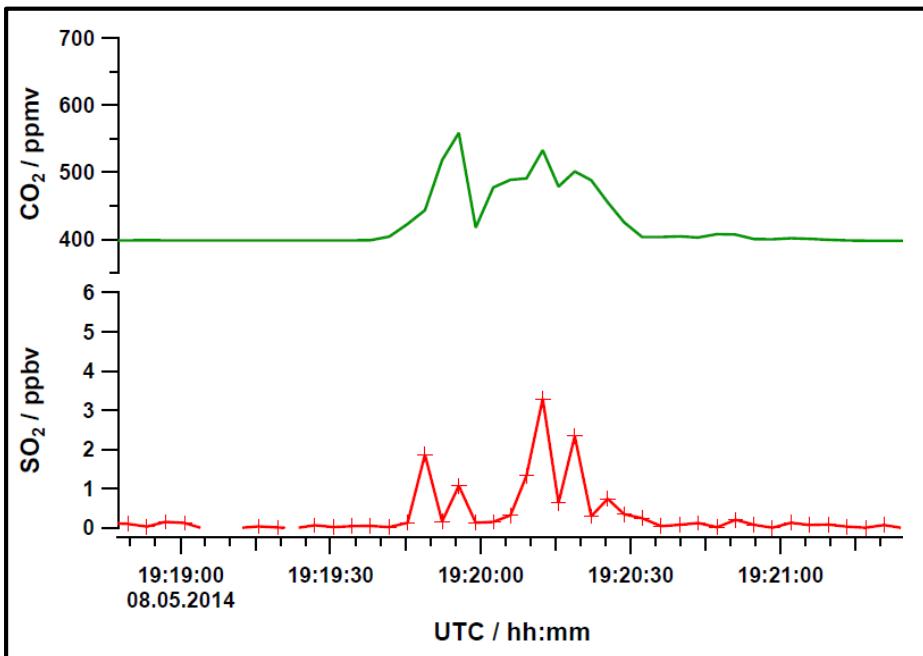
Detection limit: 10 pptv



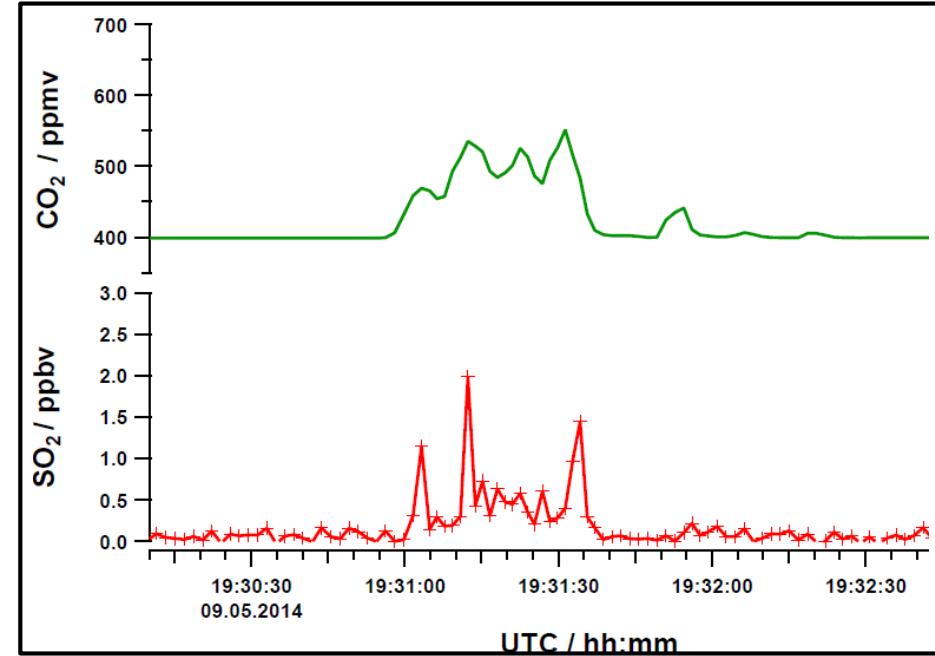
# SO<sub>2</sub> and CO<sub>2</sub> time series (flight test: May 9, 2014)



# Examples of exhaust plume sampling



May 8, 2014 / HEFA blend



May, 9, 2014 / Low S Jet A

$$EI_{SO_2} = \frac{\text{int}[SO_2] \ M_{SO_2}}{\text{int}[CO_2] \ M_{CO_2}} \ EI_{CO_2}$$

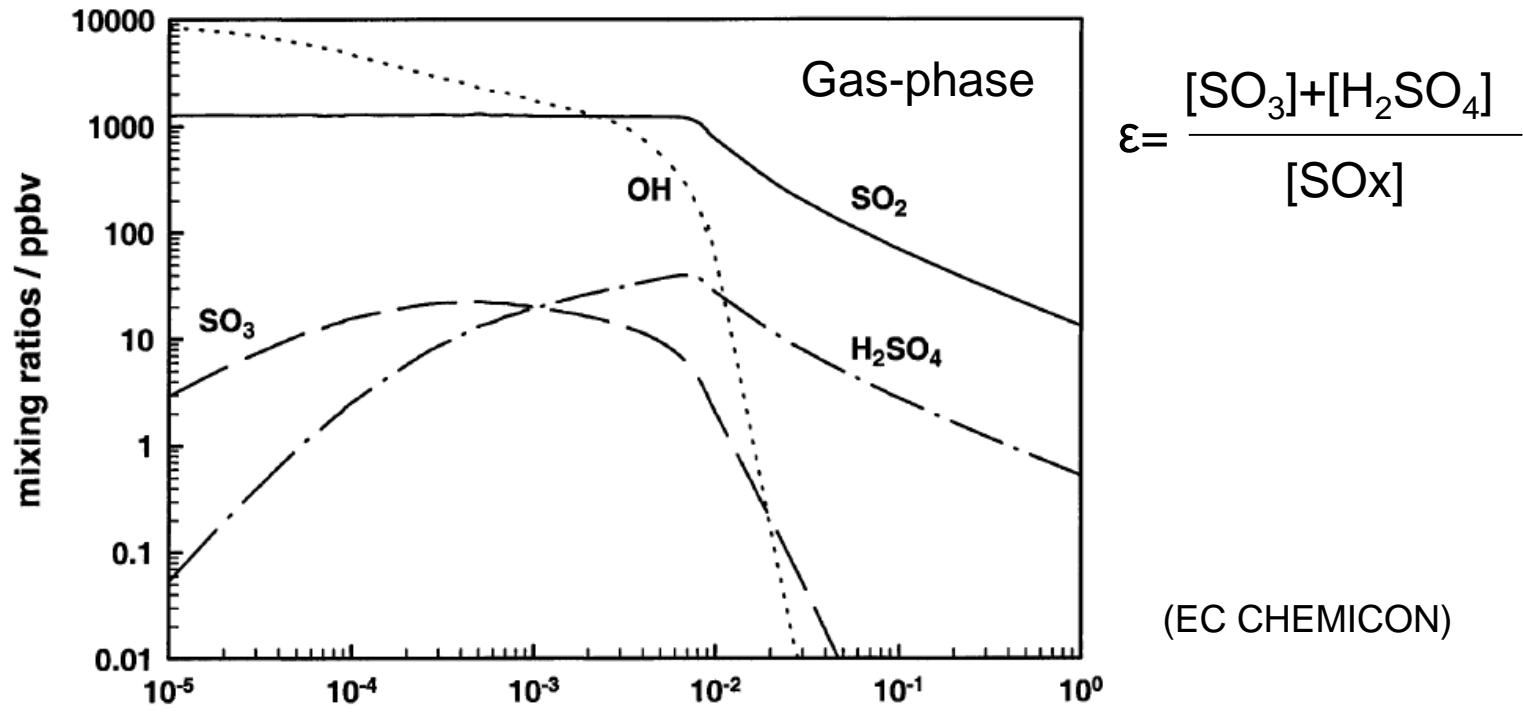


# Inferred SO<sub>2</sub> emission factors and fuel sulfur content - consistency with fuel analysis from DC8 tank

Fuel	EI (mg/ kg fuel) Flight test	FSC (ppmm) Flight test	FSC (ppmm) Fuel analysis DC8 tank2	FSC (ppmm) Fuel analysis Fuel tanker
Standard Jet A	443	221	220	--
Low S Jet A	32.4	16.2	20	9
HEFA Blend	39.7	19.9	--	16



# Sulfur conversion efficiency ( $\epsilon$ )



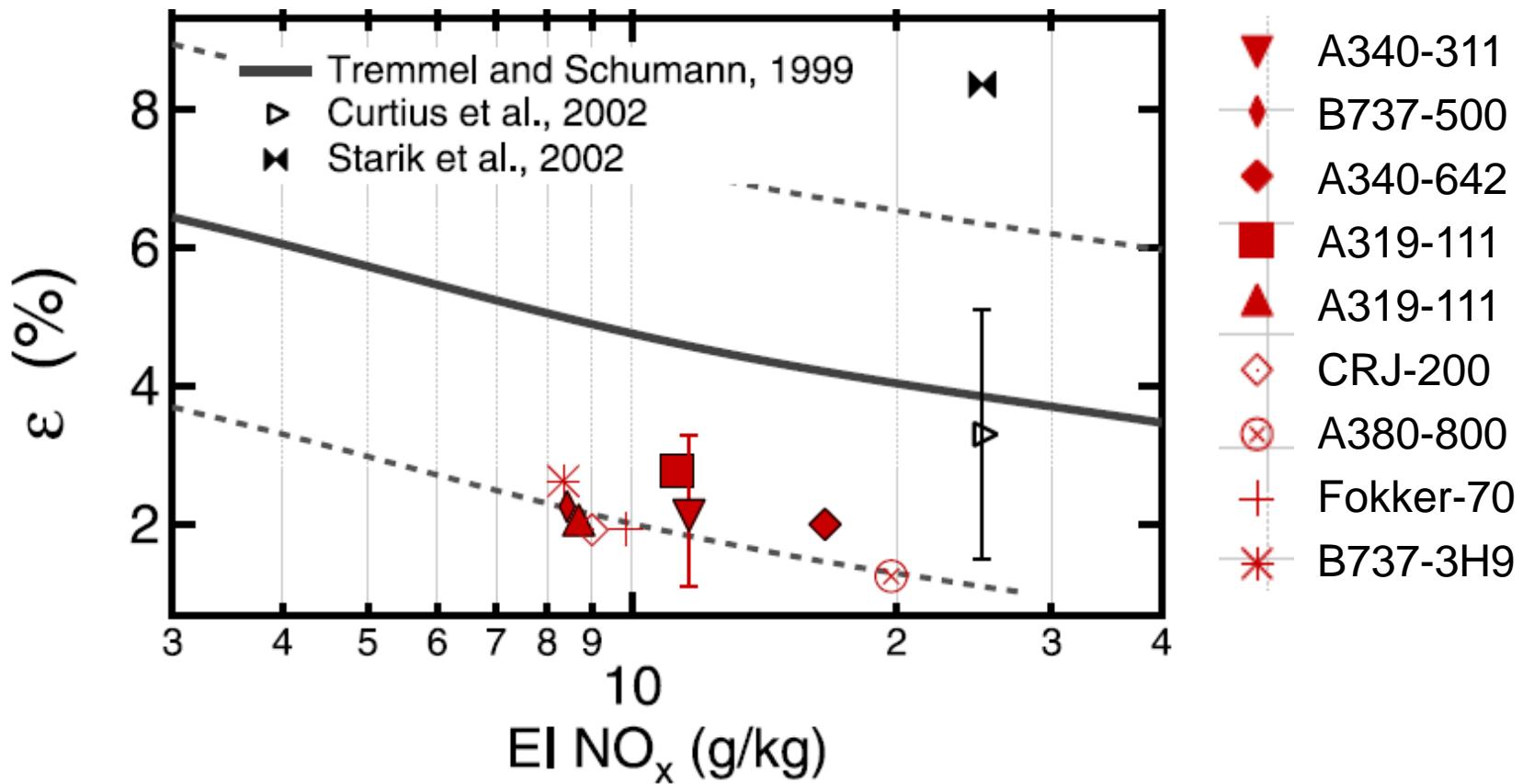
Sulfur conversion  
in combustor  
 $(\epsilon = 0.5 - 1 \%)$

Sulfur conversion  
in the flow between  
combustor and  
engine exit  
 $(\epsilon = 4 - 9 \%)$

Minor further sulfur conversion  
to  $H_2SO_4$ ,  
 $H_2SO_4$  uptake in sulfate aerosol, soot  
and ice particles

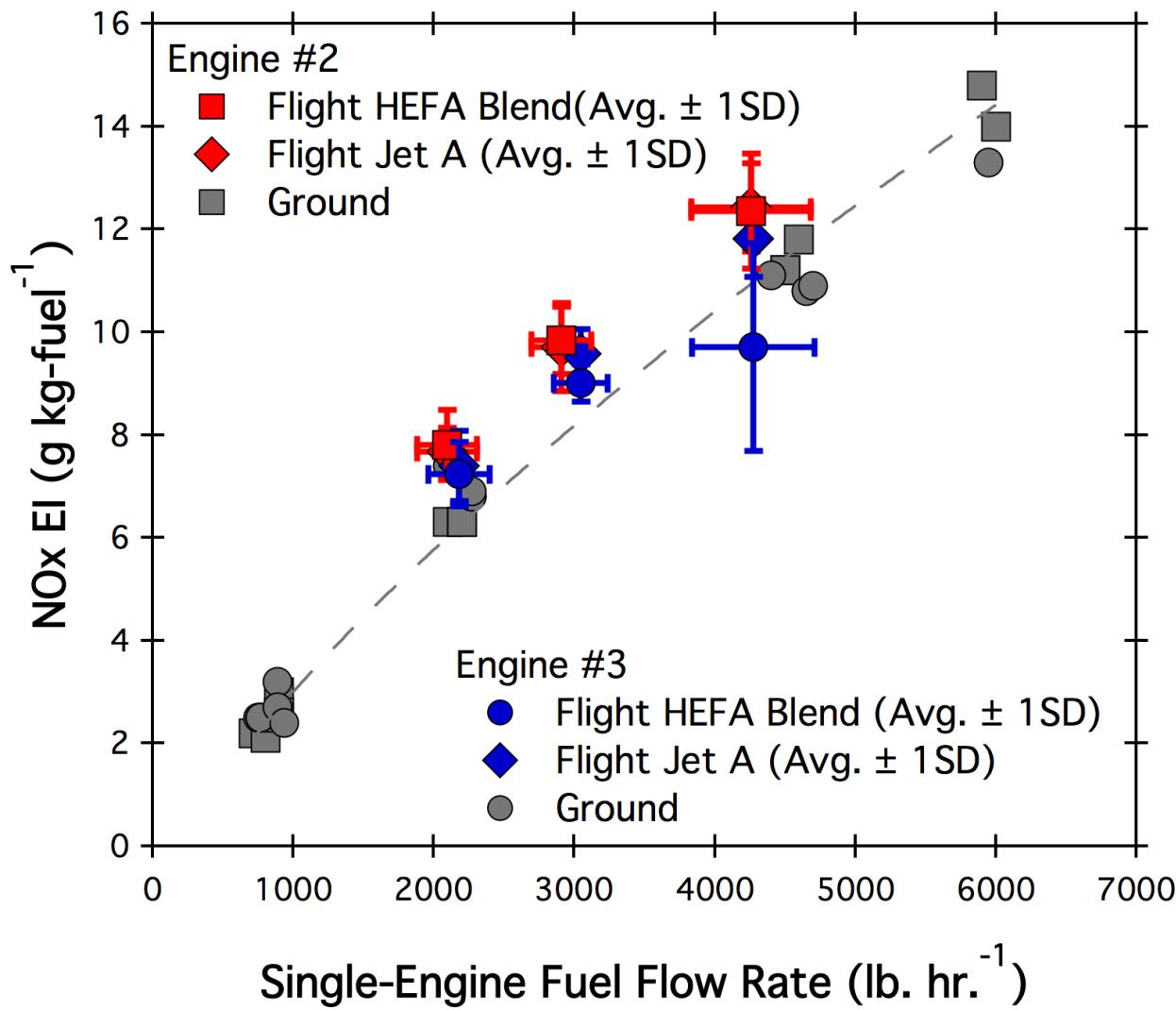


## Sulfur conversion efficiency



(Jurkat et al. 2011)

# NOx emission indices from flight and ground test



# $\text{H}_2\text{SO}_4$ IT-CIMS measurement technique



$$[\text{H}_2\text{SO}_4] = (1/k t_r) \ln(1-R), \quad R = \text{HSO}_4^-/\text{NO}_3^- \text{ cluster ions}$$

$k(h=0-2)$  measured by Viggiano et al (1997):

$2.0 \times 10^{-9} \text{ cm}^3/\text{s}$  ( $h=1$ )

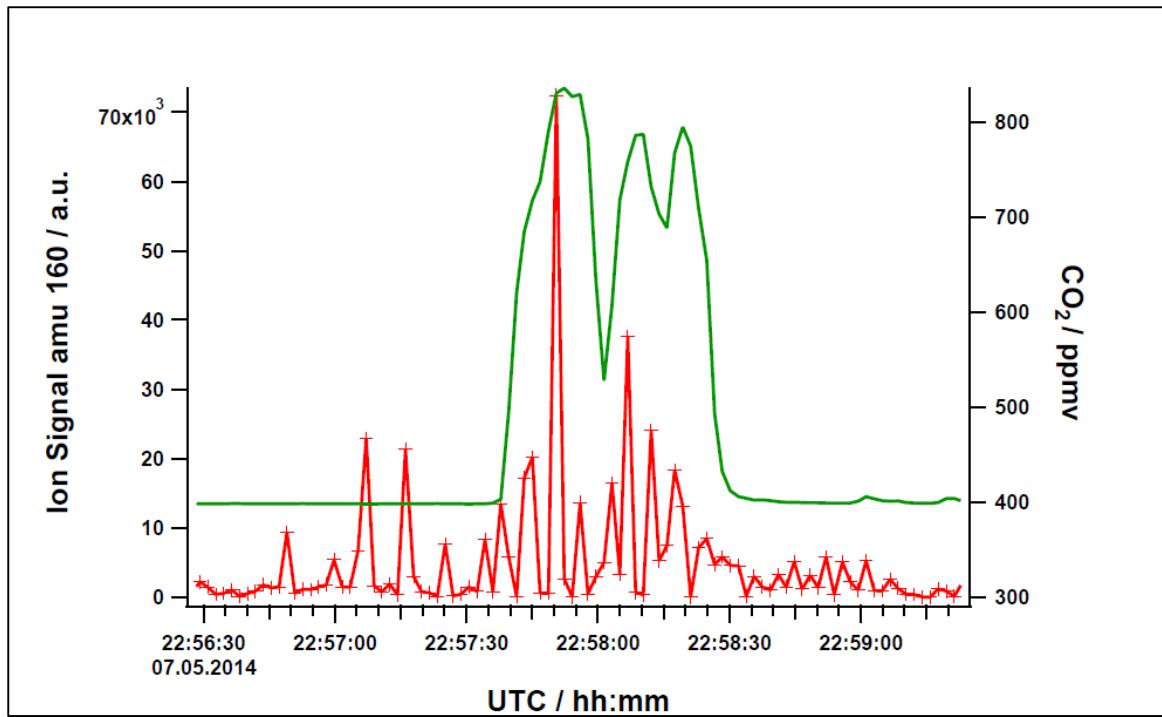
$t_r$ : drift time in reaction cell (110 ms)

Optional heated inlet section for analysis  
of total  $\text{H}_2\text{SO}_4$

DLR Falcon  
IT-CIMS



# $\text{H}_2\text{SO}_4$ and $\text{CO}_2$ measurements during flight test May 7, 2014



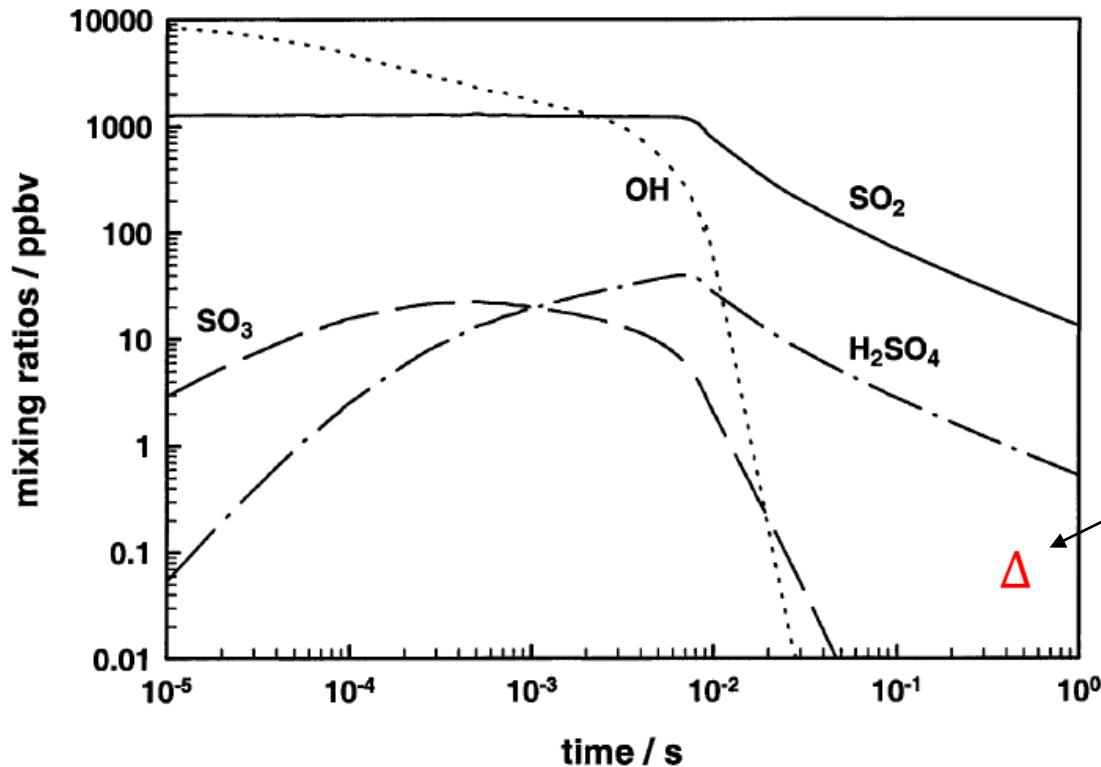
$$[\text{H}_2\text{SO}_4] = 4.7 \times 10^8 \text{ cm}^{-3}$$

$$\text{VMR}(\text{H}_2\text{SO}_4) = 50.3 \text{ pptv}$$

Plume age: 0.7s



# Sulfur conversion efficiency ( $\epsilon$ )



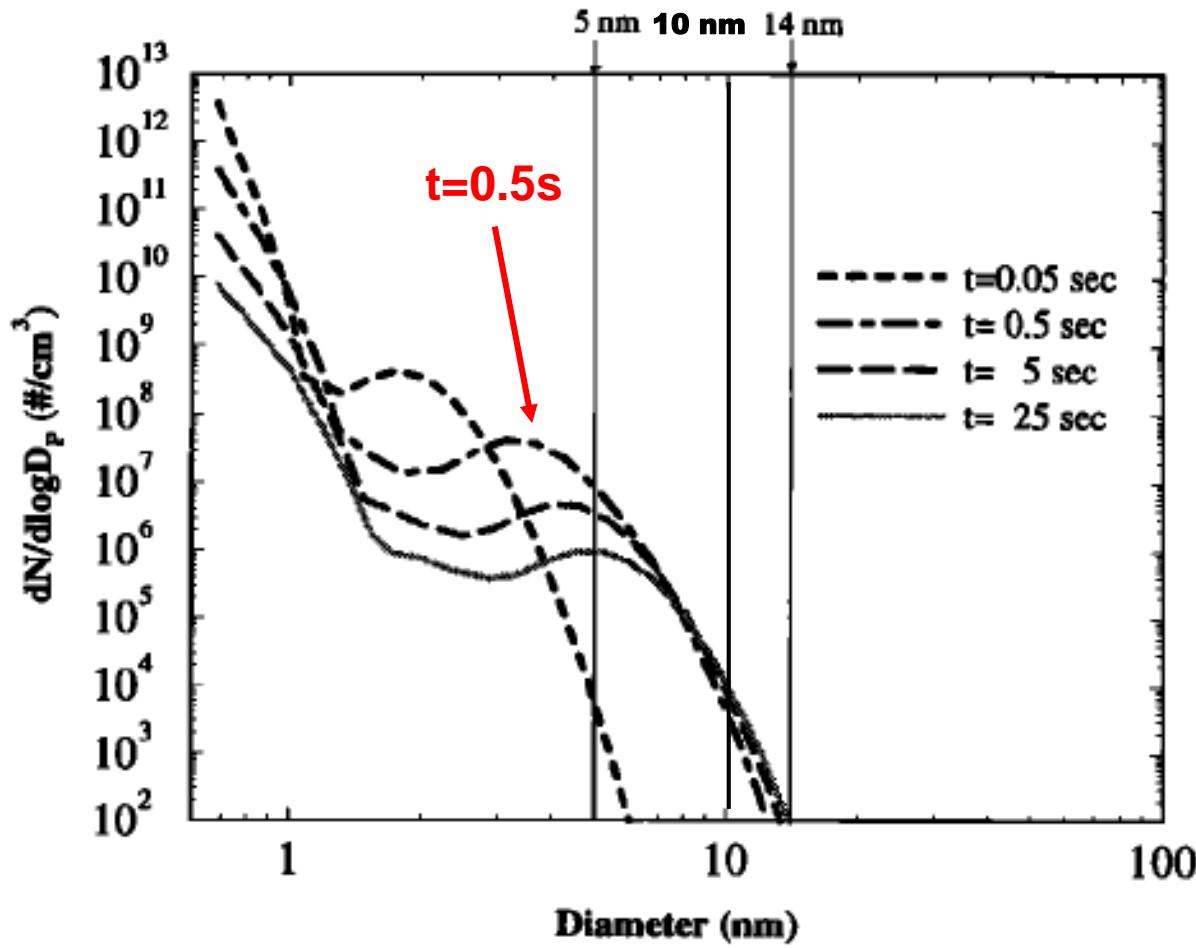
$$\epsilon = \frac{[\text{SO}_3] + [\text{H}_2\text{SO}_4]}{[\text{SOx}]}$$

ACCESS-II:  
 $\epsilon$  from detection of  
 $\text{H}_2\text{SO}_4$  gas: 0.12

->  $\text{H}_2\text{SO}_4$  mainly  
in uptake by  
particles



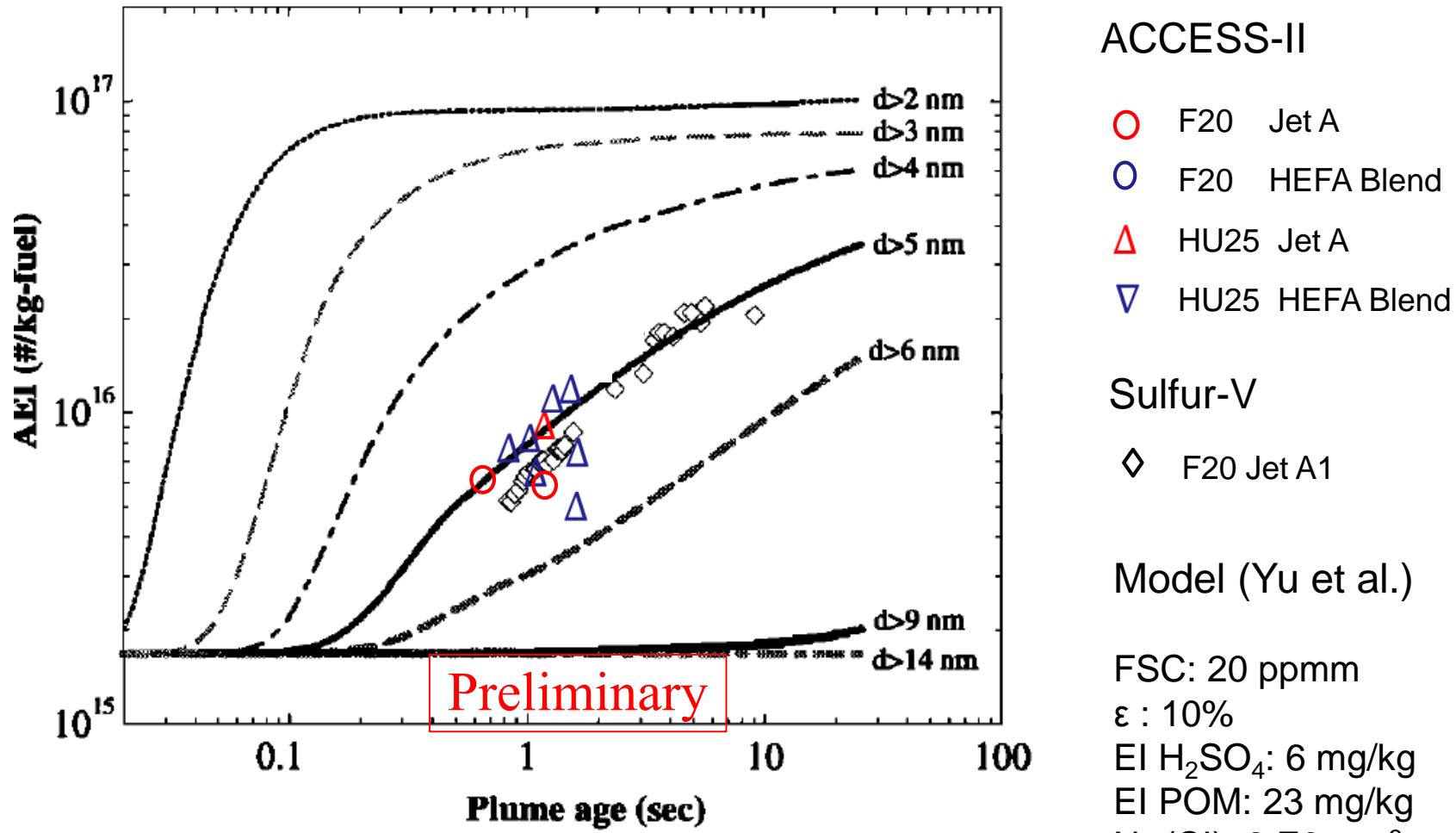
# Number size distribution of total volatile particles



FSC: 20 ppmm  
 $\epsilon$  : 10%  
EI H<sub>2</sub>SO<sub>4</sub>: 6 mg/kg  
EI POM: 23 mg/kg  
 $N_0$  (Cl): 2 E9 cm<sup>-3</sup>

(Yu et al., 1999)

# Measured and computed apparent EI of number of volatile particles (for different CPC cutoff sizes)



# Measurements of hydrocarbons with AIMS

## Measured Parameters

- Gaseous hydrocarbon compounds (HC):  
Pentene-1, Propene, Benzene, C3-Benzene,  
C4-Benzene, Phenol, Toluene, Benzaldehyde, Aceton

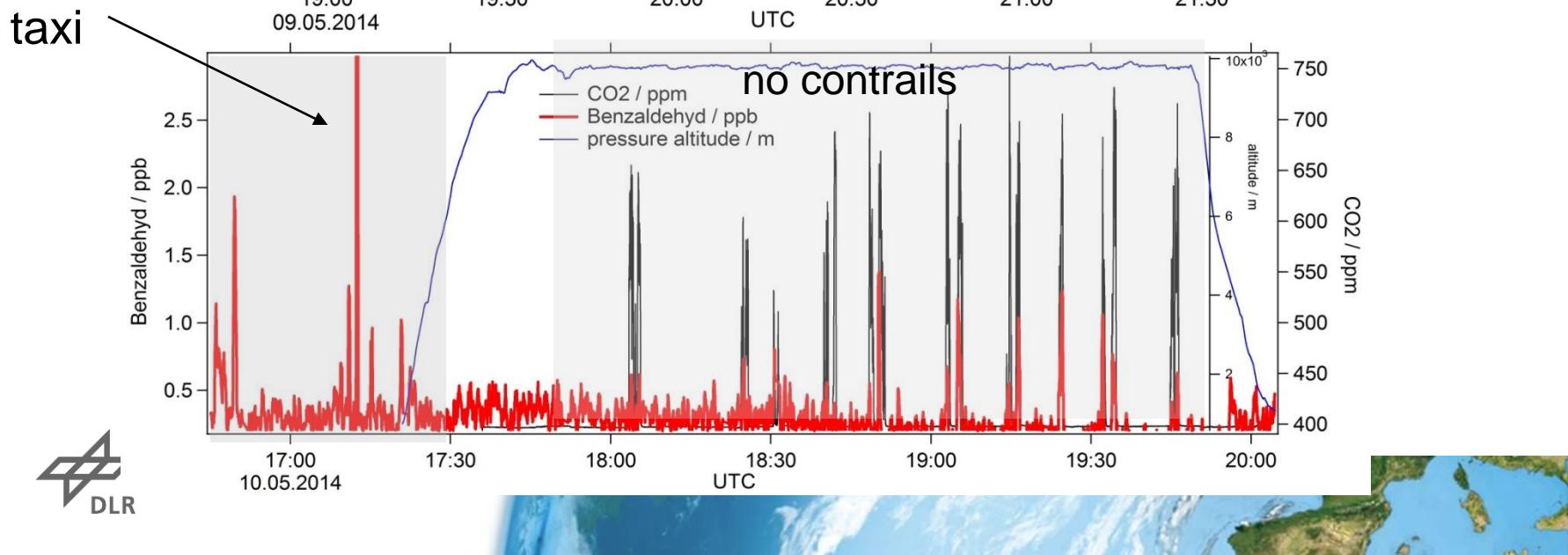
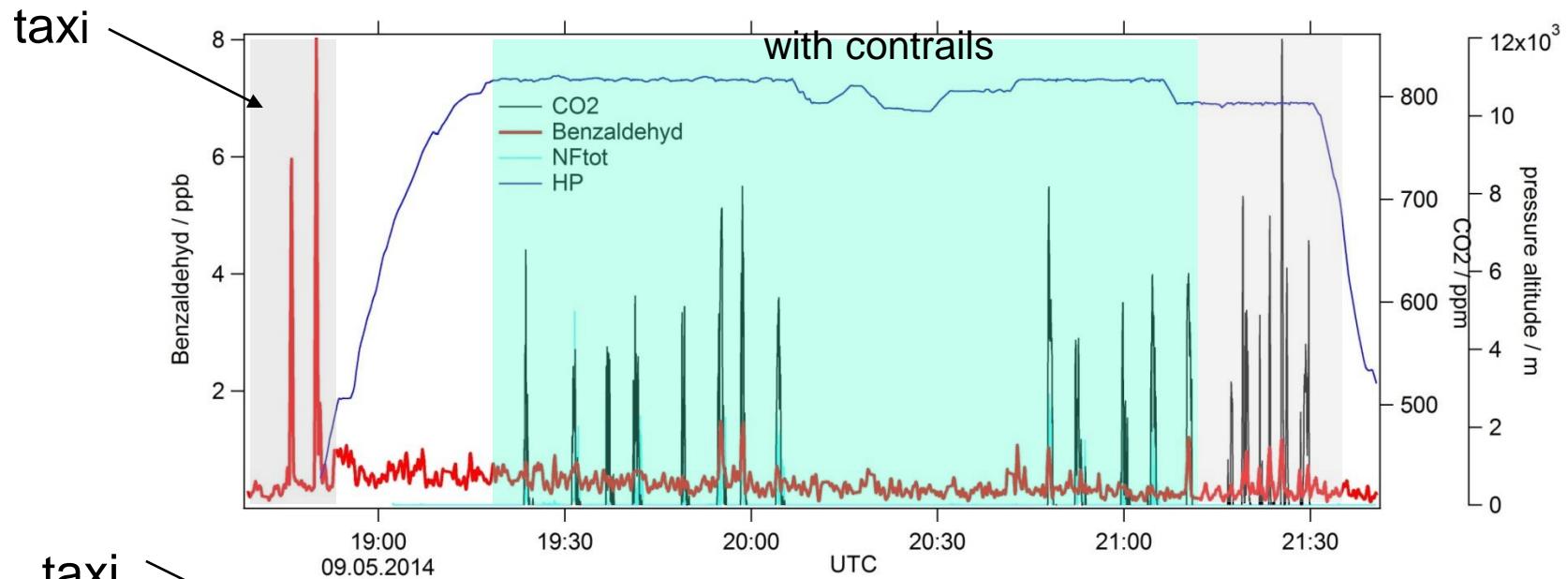
## Principal of Measurement

- Chemical ionization mass spectrometer operated in positive ion mode
- Linear quadrupole MS 0 -300 amu
- Educt ions  $\text{H}_3\text{O}^+(\text{H}_2\text{O})_n \rightarrow$  PTR- MS like mode
- Products form by proton transfer reactions

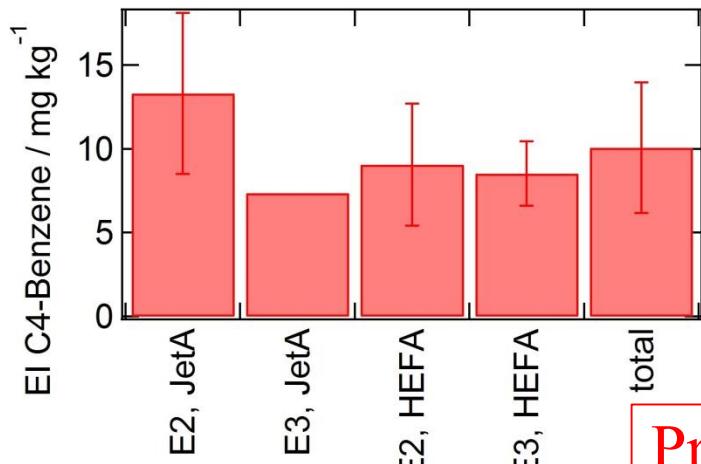


AIMS in Falcon cabin

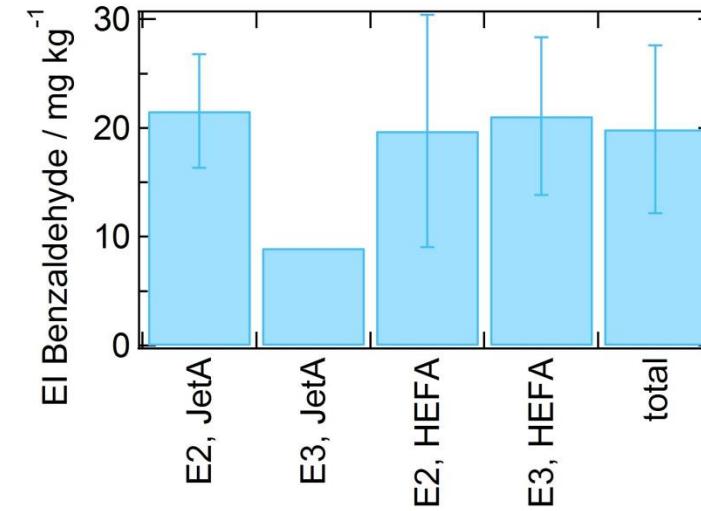
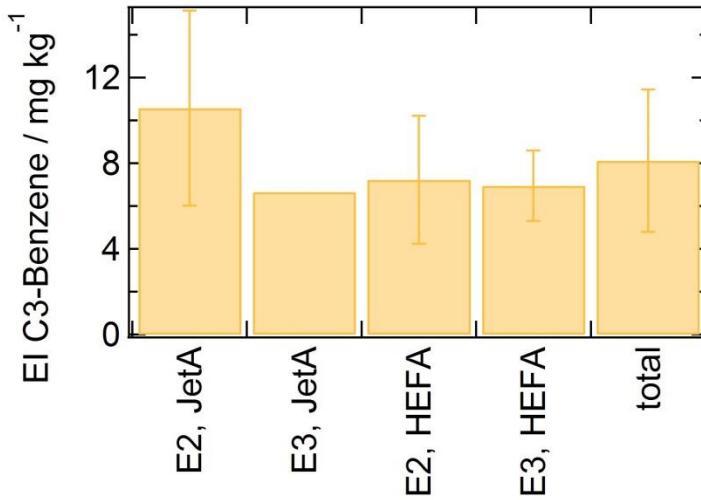
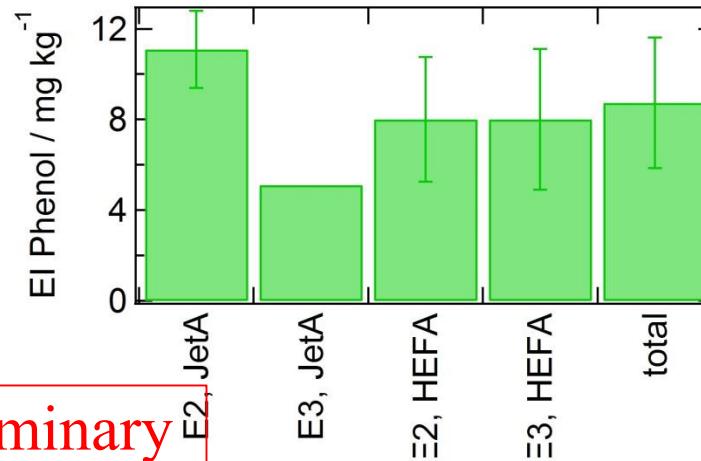
# In-flight measurements in benzaldehyd emissions



# NMHC emmission indices for non-contrail case



Preliminary



## Preliminary conclusions

- FSCs determined from flight tests agree with analysis of fuel samples within combined errors
- Sulfuric acid converted from fuel sulfur is mainly (98%) in the particle-phase in the young plumes
- No significant difference is observed for volatile particles (> 5 nm) emission factors of Jet A and HEFA blend fuels
- Emission factors of measured HC are not significantly different for Jet A and HEFA blend fuels

